



# Materials & Related Scorings

Advanced FLUKA Course

# Material under irradiation

- The prediction of the structural damage to materials under irradiation is essential to evaluate consequences due to long term employment of construction materials in nuclear reactors and charged particle accelerators.
- There are several effects and quantities that are important for studying the material behavior under irradiation and FLUKA is capable in predicting several of them:
  - Heating total energy deposition  
→ could be used for temperature rise, stresses, deformations ...
  - Energy deposition due to EMF → radiolysis calculations ...
  - Dose calculation → medical applications ...
  - Gas production
  - Non Ionizing Energy Losses (NIEL) ] → material damage ...
  - Displacement per Atoms (dpa)
  - Silicon 1MeV Neutron Equivalent (Si1MeVEq) ] → electronics
  - Single Event Upsets to electronics (SEU)

*For all the above you need to input the proper MATERIAL properties*

# Material definition

## Single-element material definition

	atomic number Z	atomic weight	density (g/cm <sup>3</sup> )	material number	Alternate material to use for dE/dx	mass number (A)	name
* . . . + . . . 1 . . . + . . . 2 . . . + . . . 3 . . . + . . . 4 . . . + . . . 5 . . . + . . . 6 . . . + . . . 7 . . . + . . .							
MATERIAL	24.0	51.9961	7.18	26.0	0.0	0.0	CHROMIUM
MATERIAL	Z: 15	Name: PHOSPHO Am: 30.973761		# A:		ρ: 2.2 dE/dx: ▼	

### Notes:

- if  $\rho < 0.01$ : gas at atmospheric pressure
- Atomic Weight is **calculated by the code** using the internal database is better to leave empty
- Material number use it **ONLY** if you want to **override** a predefined one
- Mass Number to define specific **ISOTOPES**  
*Do not confuse with the Atomic weight*
- Choose a name corresponding to the **LOW-ENERGY neutron database** Section 10.4 in the manual

# Predefined ICRU materials

In the present version of FLUKA, the code contains several predefined materials with the composition suggested by ICRU

FLUKA	Material	FLUKA	Material
AIR	Dry air 20°C	BONECOMP	Compact bone
WATER	Water	BONECORT	Cortical bone
POLYSTYR	Polystyrene	MUSCLESK	Skeletal muscle
PMMA	Polymethyl methacrylate	MUSCLEST	Striated muscle
POLYETHY	Polyethylene	ADTISSUE	Adipose tissue
PLASCINT	Plastic scintillator	KAPTON	Kapton

- The materials can be used WITHOUT the need of an explicit MATERIAL / COMPOUND cards
- If the user defines a MATERIAL card in the input with the same name as the predefined ones IT WILL OVERRIDE THE PREDEFINED.

# Material Assignment

A (single-element or compound) material is assigned to each geometry region.

*...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...	MATERIAL	from REGION	to REGION	step	magnetic field	MATERIAL for decay run
ASSIGNMA	GOLD	TARGS1	TARGS3	1.0	0.0	BLCKHOLE
ASSIGNMA	Mat: WATER ▼	Reg: WATERCNT ▼	to Reg: ▼			
	Mat(Decay): BLCKHOLE ▼	Step:	Field: ▼			

In the new version of FLUKA:

- **WHAT(5)** is controlling the magnetic (& electric) field for the prompt and radioactive decay product transport
- **WHAT(6)** is permitting to assign a different material for the radioactive decay product transport.

# MAT-PROP

Card: MAT-PROP

<b>MAT-PROP</b>	Type: ▼	Gas pressure:	RHOR:
Ionization:	Mat: ▼	to Mat: ▼	Step:

- Supply extra information on gaseous materials (pressure)
- Create materials with fictitious or effective density
- Override the default ionization potential

<b>MAT-PROP</b>	Type: DPA-ENER ▼	DPA Eth:	
	Mat: ▼	to Mat: ▼	Step:

- Set the **DPA** energy damage threshold (WARNING in **eV**)

<b>MAT-PROP</b>	Type: USERDIRE ▼	Call: USRMED ▼	
	Mat: ▼	to Mat: ▼	Step:

- Enable the call to **USRMED** routine when a particle enters in the desired materials

There is a last option **LOWNTEMP** to change the material temperature for the new treatment at thermal energies. **HOWEVER** *it cannot be applied with the new library with 260 groups*

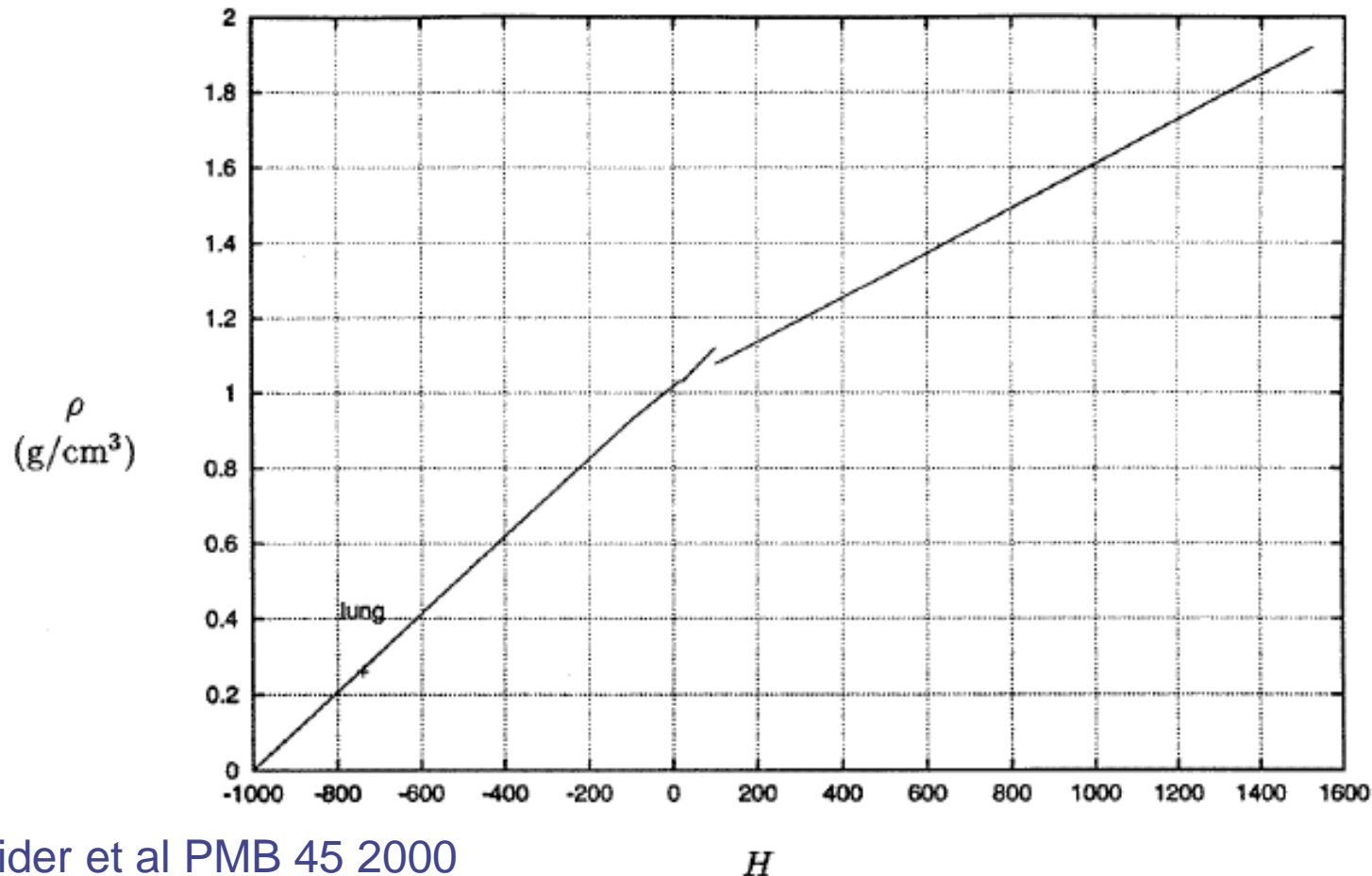
# CORRFAC: Region dependent – 1

<b>CORRFAC</b>	xp (dE/dx):	xp other:	
	Reg: ▼	to Reg: ▼	Step:

- **CORRFAC** card allows to alter material density for dE/dx and nuclear processes
- First two inputs specify a **density scaling factor** (restricted to the interval [2/3,3/2]) for **charged particle ionization processes** (**WHAT(1)**) and for all other processes (**WHAT(2)**) to the region(s) specified by the inputs **WHAT(4-6)**
- If **WHAT(1)<0**. then it is relative to the density scaling:  
**scaling factor = |WHAT(1)|×WHAT(2)**
- This is especially important in ion beam therapy to force the MC to follow the same **semi-empirical Hounsfield Units-range calibration curve** as the Treatment Planning System (TPS) for dosimetric comparisons.
- Typically, a user has to deal with a CT stoichiometric calibration, i.e. a **segmentation of the CT** scan (expressed in Hounsfield units (HU)) into materials of defined elemental composition (for example Schneider *et al* 45 2000).

# CORRFAC: Region dependent – 2

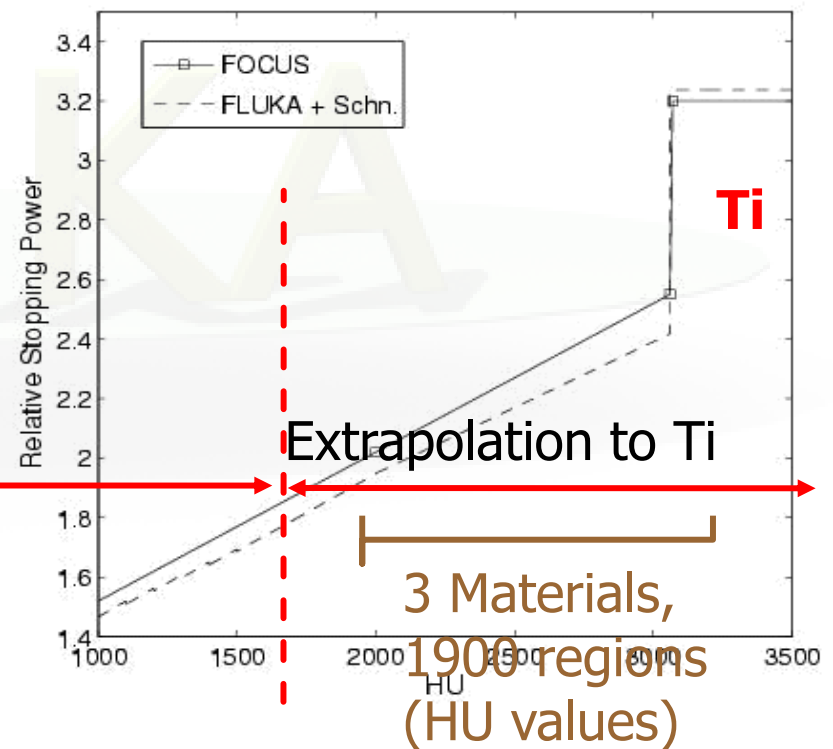
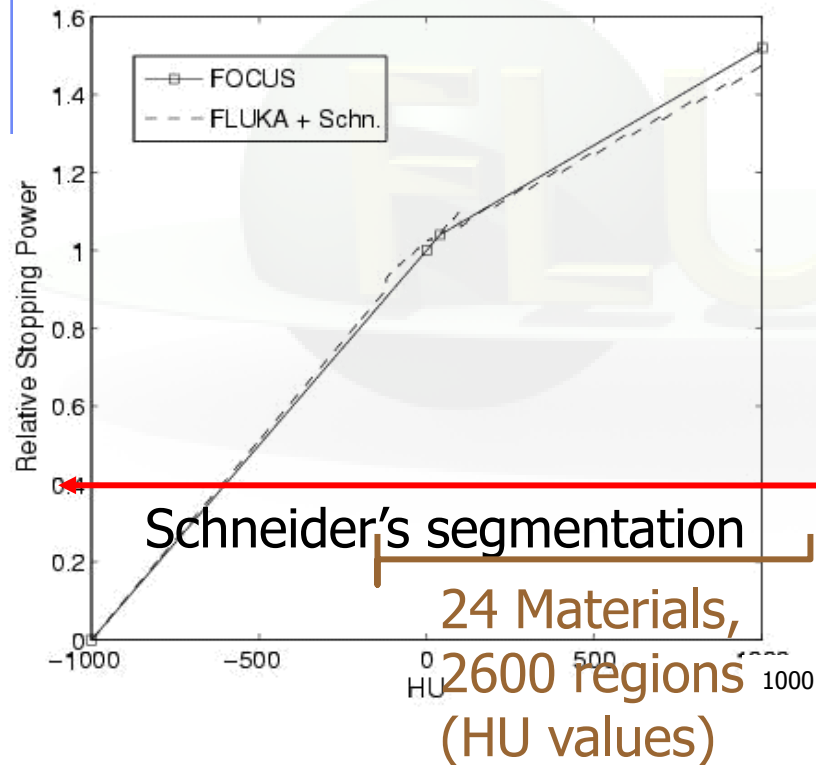
- A “nominal density”, e.g., using the density at the center of each HU interval (Jiang et al MP 2004) is assigned to each material. But “real density” (and related physical quantities) varies continuously with HU values.





# FLUKA forced to follow the same range calibration curve as TPS for protons @ MGH

The CORRFACT ionization scaling factors (WHAT(2) in the CORRFACT card) were obtained from the ratio between TPS and FLUKA (+Schneider et al “mass” density)



Parodi et al MP 34, 2007, Parodi et PMB 52, 2007

# STERNHEI me card

<b>STERNHEI</b>	Cbar:	X0:	X1:
Mat: ▼	a:	m:	$\delta 0$ :

- Below the  $\delta$ -ray threshold, energy losses are treated as “continuous”, with some special features:
  - Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
  - The energy dependence of cross sections and dE/dx is taken into account exactly
  - Latest recommended values of ionization potential and density effect parameters implemented for elements (Sternheimer, Berger & Seltzer), but can be overridden by the user with (set yourself for compounds!) the

STERNHEI C X0 X1 a m  $\delta 0$  MAT

- In addition, the card MAT-PROP can be used a to override the value of the average ionization potential used by the program

MAT-PROP Gasp Rhosc Iion Mat1 Mat2 Step

# dpa: Displacements Per Atom

- Is a measure of the amount of radiation damage in irradiated materials  
*For example, 3 dpa means each atom in the material has been displaced from its site within the structural lattice of the material an average of 3 times*
- Displacement damage can be induced by all particles produced in the hadronic cascade, including high energy photons. The latter, however, have to initiate a reaction producing charged particles, neutrons or ions.
- The dpa quantity is directly related with the total number of defects (or Frenkel pairs)

$$dpa = \frac{1}{\rho} \sum_i N_i N_f^i$$

$\rho$  atoms/cm<sup>3</sup>

$N_i$  particles per interaction channel  $i$

$N_f^i$  Frenkel pairs per channel

# Frenkel pairs

- Frenkel pairs  $N_F$  (defect or disorder), is a compound crystallographic defect in which an **interstitial** lies near the **vacancy**. A Frenkel defect forms when an atom or ion leaves its place in the lattice (leaving a vacancy), and lodges nearby in the crystal (becoming an interstitial)

$$N_{NRT} \equiv N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

$N_{NRT}$   
 $\kappa=0.8$   
 $T$

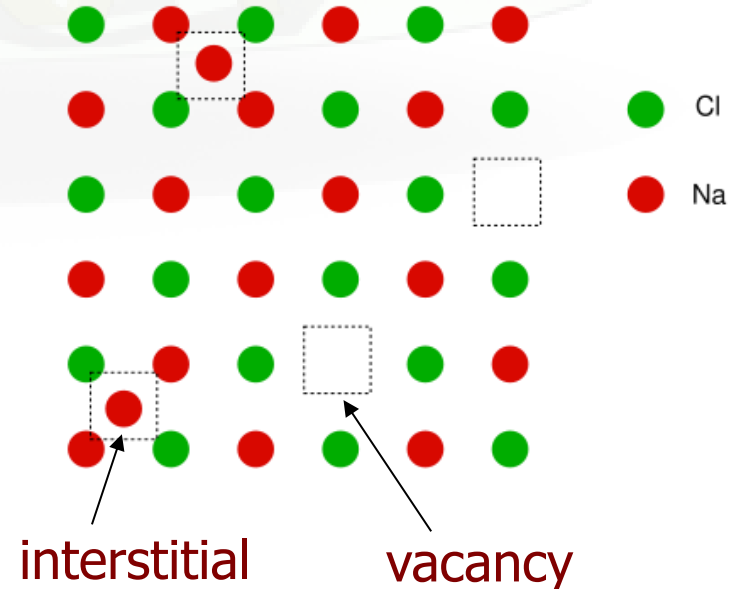
Defects by Norgert, Robinson and Torrens  
 is the displacement efficiency  
 kinetic energy of the primary  
 knock-on atom (PKA)

$\xi(T)$   
 $\xi(T) T$

partition function (LSS theory)  
 directly related to the **NIEL**  
 (non ionizing energy loss)

$E_{th}$

damage threshold energy



$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

# $E_{th}$ Damage Threshold Energy

- $E_{th}$  is the value of the threshold displacement energy averaged over all crystallographic directions or a minimum energy to produce a defect

Element	$E_{th}$ (eV)	Element	$E_{th}$ (eV)
Lithium	10	Co	40
C in SiC	20	Ni	40
Graphite	30..35	Cu	40
Al	27	Nb	40
Si	25	Mo	60
Mn	40	W	90
Fe	40	Pb	25

Typical values used in NJOY99 code

- FLUKA way

**MAT-PROP**    *WHAT(1)*            =  $E_{th}$  (eV)  
                           *WHAT(4,5,6)*        = Material range  
                           *SDUM*                        = **DPA-ENER**

# FLUKA Implementation [1/2]

## Charged particles and heavy ions

### • During Interactions

- ✓ ■ For all charged particles and Heavy Ions, calculate the recoil.  
Use recoil as a normal particle

### • During transport

- ✓ ■ Calculate the restricted and unrestricted nuclear stopping power for the average energy at the middle of the step with calls to DEDXNU and SNRDFR and add it to TKNIEL and TKEDPA global variables
- ✗ ■ For electrons Bremsstrahlung, sample randomly a recoil energy from the distribution of the recoils (uncorrelated with the event)  
Treat the recoil as a normal particle (*work on progress*)

### ✓ Below threshold

- Calculate the TKNIEL(=TKEDPA) by using the Lindhard partition function

# FLUKA Implementation [2/2]

## Neutrons

- **High energy  $E_n > 20$  MeV**

- ✓
  - Like CP, **calculate the recoil**.  
Treat recoil as a normal particle

- **Low energy  $E_n \leq 20$  MeV (group-wise)**

- ✓
  - Calculate the NIEL from NJOY, then add it to **TKNIEL** and **TKEDPA** global variables

- **Low energy  $E_n \leq 20$  MeV (point-wise)**

- ✗
  - Calculate the recoil if possible
- ✓
  - Treat the recoil as a normal particle  
(available for those where point-wise exist)

## Photons

- ✗
  - **Pair production**, sample randomly a recoil for a distribution  
(uncorrelated with the event) Treat the recoil as a normal particle

# dpa: Recipe

FLUKA is using a more accurate treatment during the particle transport. While below the transport threshold is employing the Lindhard approximation with the NRT model, it is strongly advisable to use as low thresholds as possible:

## **Thresholds:**

- All Hadrons 1 keV
- Neutrons down to thermal ( $1e-15$  GeV)
- Leptons 50-100 keV would be ok

## **Material Damage:**

Set with **MAT-PROP** the damage threshold for all materials under consideration. All other will use the default of **30eV!!!!**

## **Scoring:**

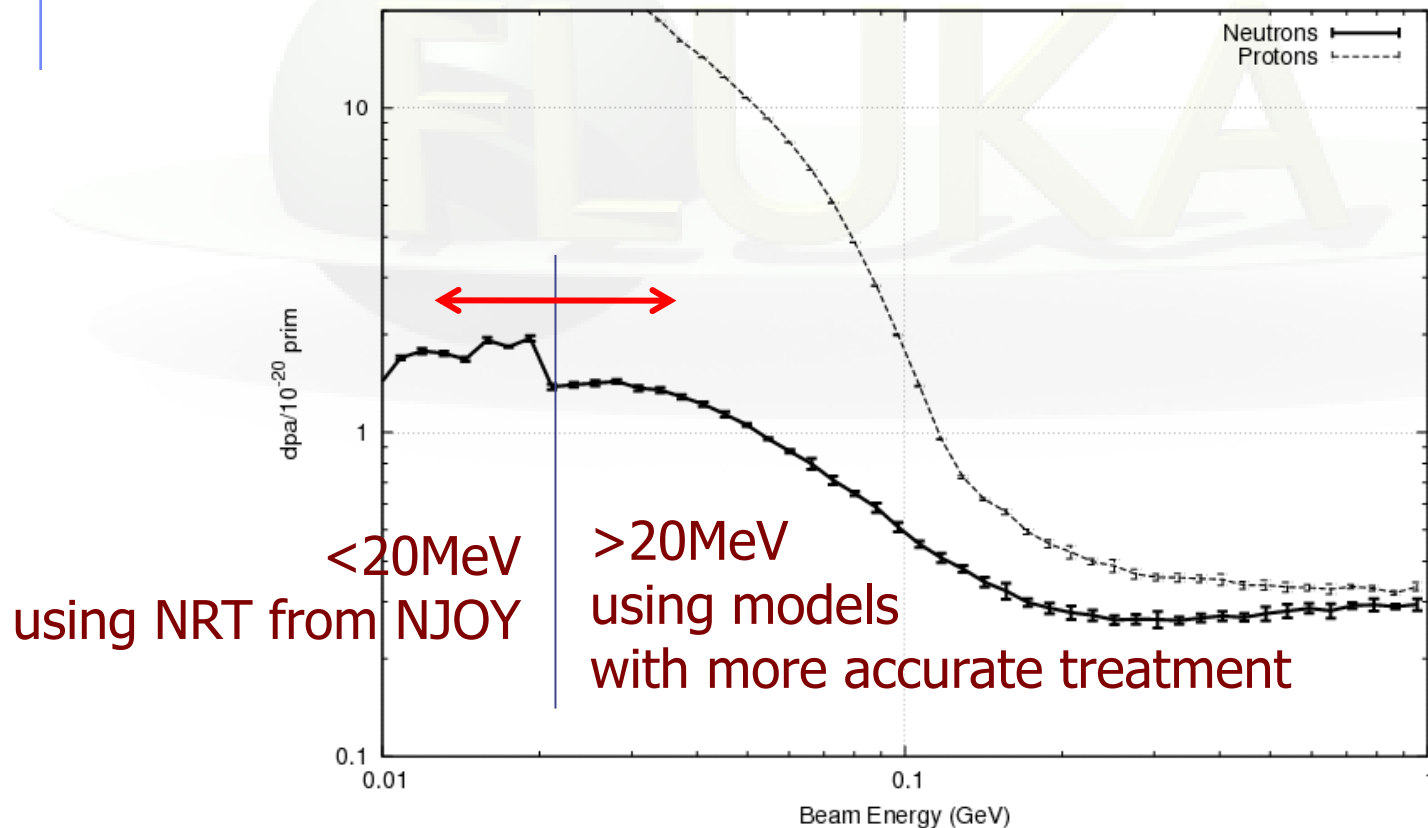
Use **USRBIN** with **DPA-SCO** or **NIEL**

**DEFAULTS: DAMAGE**



# dpa: Artifacts

- Due to the group treatment of low-energy neutrons, there is no direct way to calculate properly the recoils.
- Therefore the evaluation is based on the KERMA factors calculated by NJOY, which in turn is based on the Unrestricted Nuclear losses from using the NRT model.



# Cards Displacement Damage + Charge

For all charged particles and Heavy Ions FLUKA calculates the recoil as a normal particle. During transport it calculates the restricted and unrestricted nuclear stopping power, allowing to score dpa's and non-ionizing energy loss (NIEL):

<b>NIEL-DEP</b>	Non Ionizing Energy Loss deposition
<b>DPA-SCO</b>	Displacements per atoms

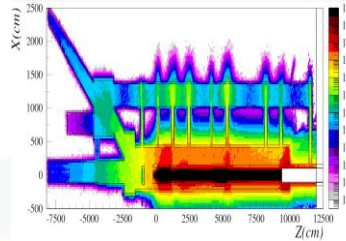
In addition (not necessarily linked to displacement damage) the following can be useful in order to get the net charge deposition in a given region:

<b>NET-CHRG</b>	Net Charge
-----------------	------------

# Radiation Physics/Effects/Monitoring

nuclear cascade

$h > 20 \text{ MeV}$



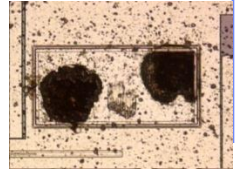
**Radiation Field**

$h, e, \dots > 100 \text{ KeV}$

*EM cascade*

radiation damage in semiconductors

*Single Events*



**Effect in the Device**

*Dose*

*Displacement*

radiation monitor



*Radfet*

*SEU counter*

**Measurement**

*PIN Diodes*



# Main Radiation Effects on Electronics

Category		Effect
<b>Single Event effects</b>  (Random in time)	<b><i>Single Event Upset (SEU)</i></b>	Memory bit flip (soft error) Temporary functional failure
	<b><i>Single Event Latchup (SEL)</i></b>	Abnormal high current state Permanent/destructive if not protected
<b>Cumulative effects</b>  (Long term)	<b><i>Total Ionizing Dose (TID)</i></b>	Charge build-up in oxide Threshold shift & increased leakage current Ultimately destructive
	<b><i>Displacement damage</i></b>	Atomic displacements Degradation over time Ultimately destructive

# Radiation Damage to Electronics

- All important quantities to estimate risks of damage to electronics can be directly scored in FLUKA :

## **Cumulative damage:**

- Energy deposition (total ionizing dose) by scoring **DOSE** with any 'energy deposition like estimator' (*e.g.*, **USRBIN**)
- Si Lattice displacement (1-MeV neutron equivalent particle fluxes) with any 'fluence like estimator' (*e.g.*, **USRTRACK**)

## **Stochastic failures (SEU):**

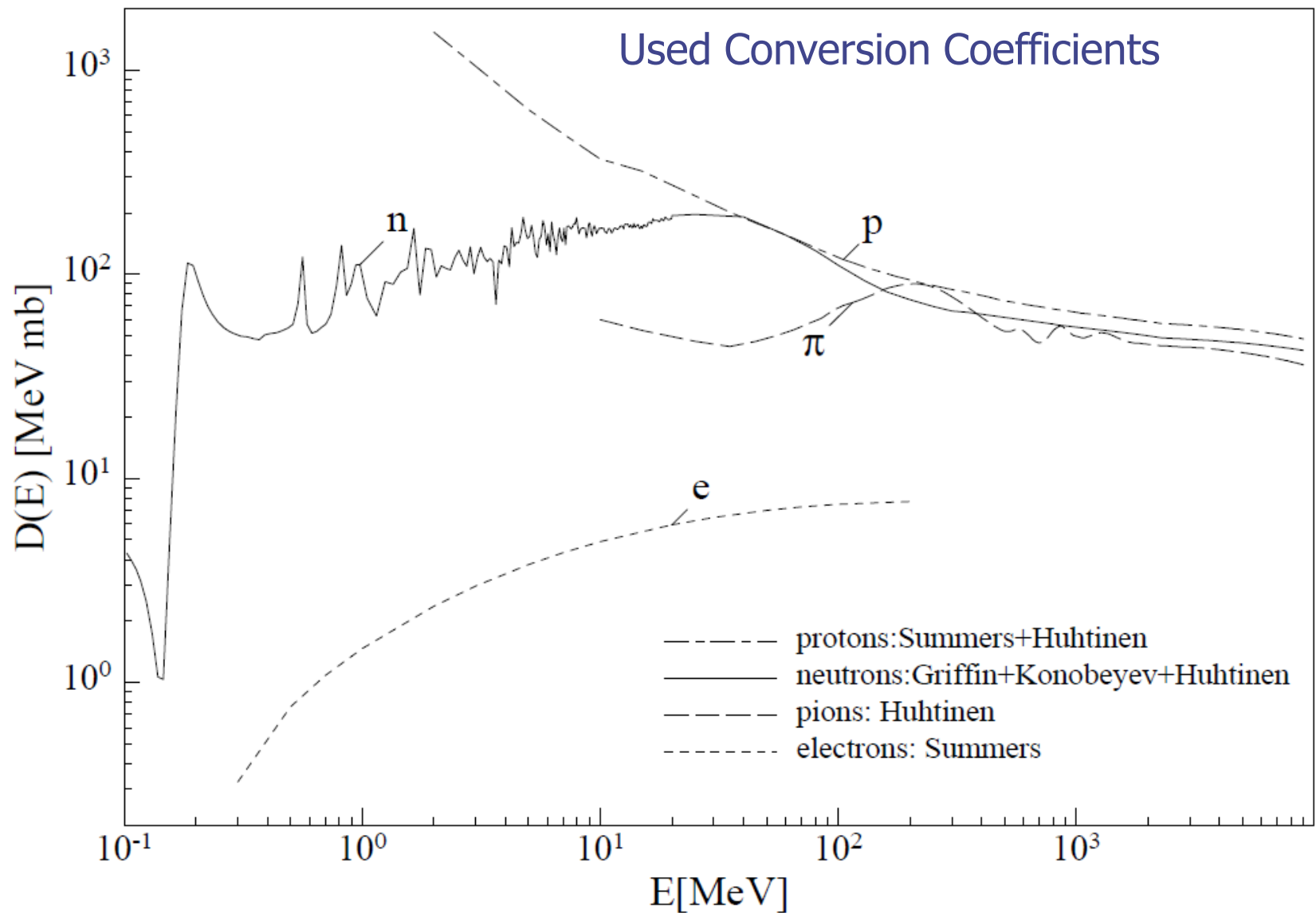
- "high" energy hadron fluences ("E>20 MeV") with any 'fluence like estimator' (*e.g.*, **USRTRACK**)  
(**the option of special threshold functions [user defined] is currently in development and will be included in the next release together with the scoring related to the "damage by thermal neutrons"**)
- The powerful FLUKA scoring options together with the analysis of particle energy spectra allows a detailed study in order to select best possible locations for electronics or efficiently design shielding implementations

# Corresponding FLUKA Estimators

Category		Scales with simulated/measured quantity
Single Event effects <i>(Random in time)</i>	<b>Single Event Upset (SEU)</b>	HADGT20M [cm <sup>-2</sup> ] (+/or HEHAD-EQ, THNEU-EQ)
	<b>Single Event Latchup (SEL)</b>	HADGT20M [cm <sup>-2</sup> ] (+/or HEHAD-EQ)
Cumulative effects <i>(Long term)</i>	<b>Total Ionizing Dose (TID)</b>	DOSE [GeV/g] -> stricly IONIZING only!
	<b>Displacement damage</b>	SI1MEVNE [cm <sup>-2</sup> ] {NIEL}

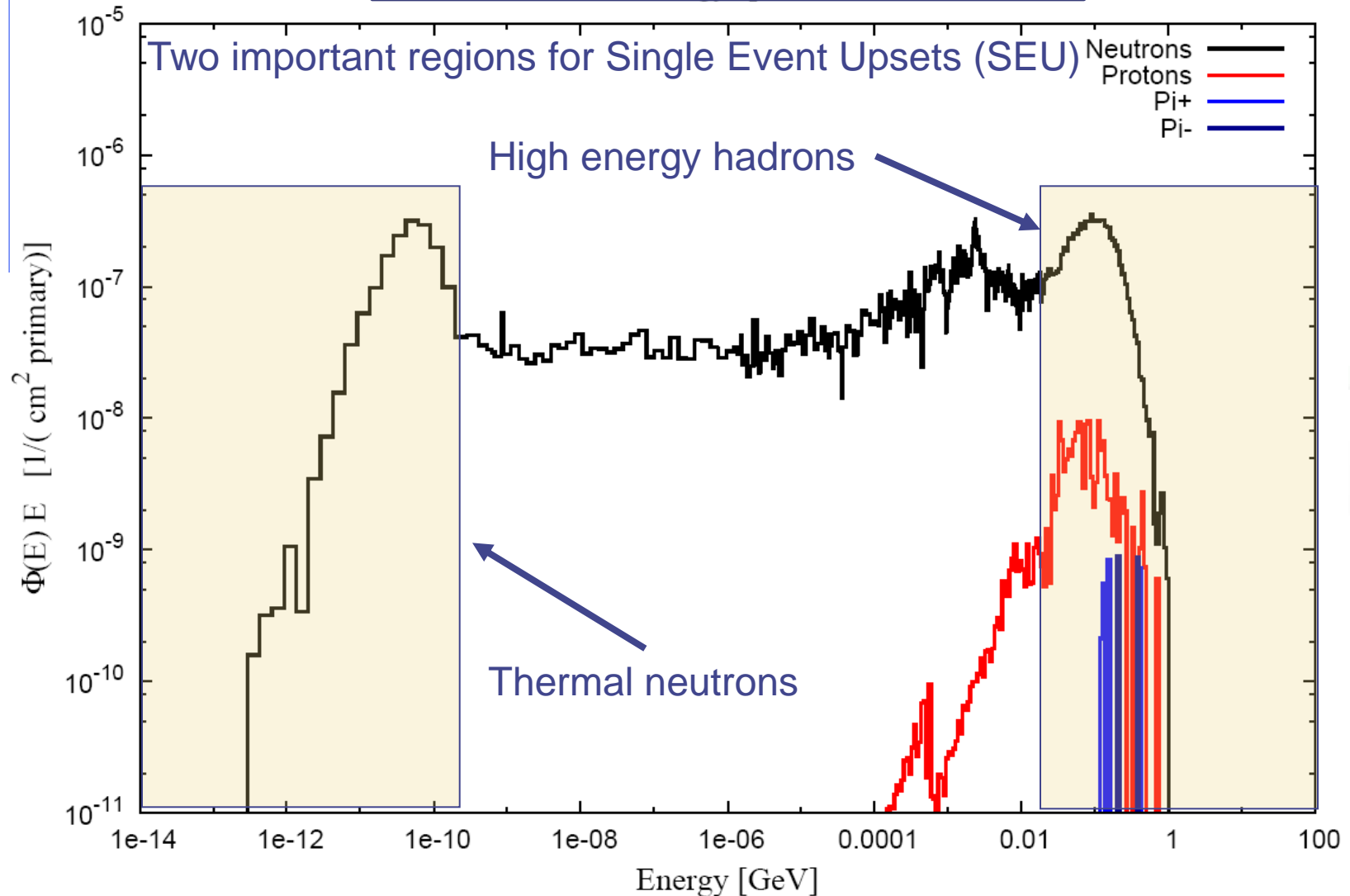
- \* Reality is more complicated (*e.g.*, contribution of thermal neutrons)
- \*\* Energy threshold for inducing SEL is often higher than 20 MeV (*e.g.*, 5-20MeV, see scoring lecture and discussion on future scoring possibility)

# 1MeV Neutron Equivalent



# SEUs in mixed radiation field

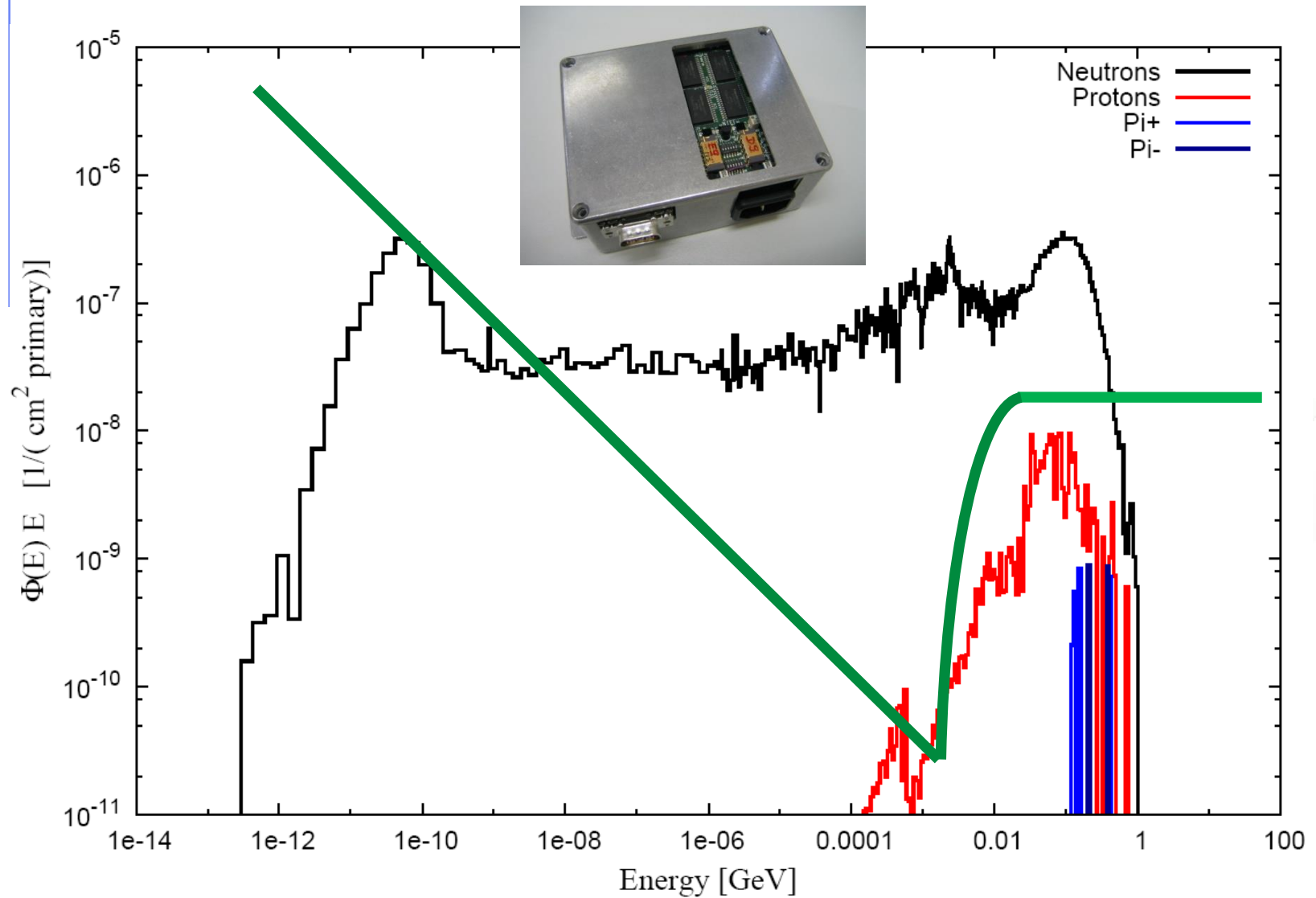
$$\#SEU = S_{Th. n.} \times F_{Th. n.} + \sigma_{HEH} \cdot \Phi_{HEH}$$



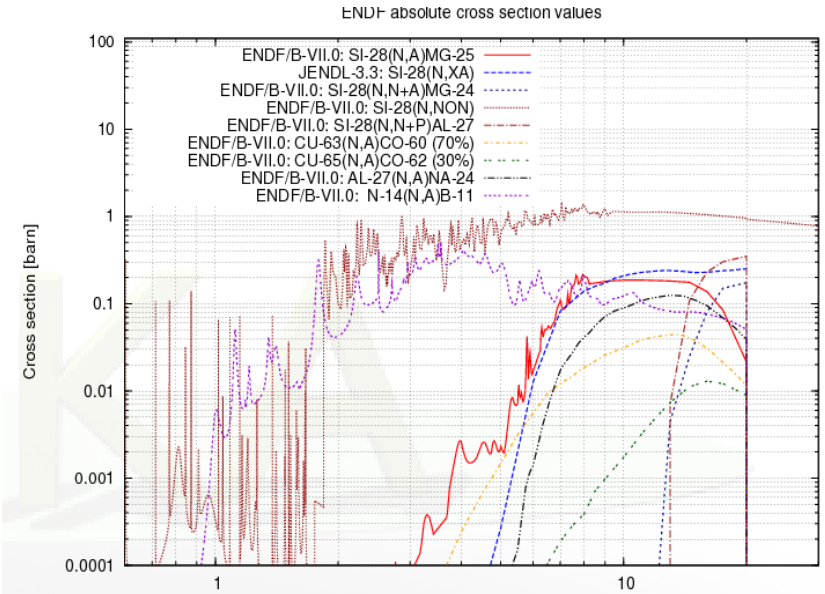
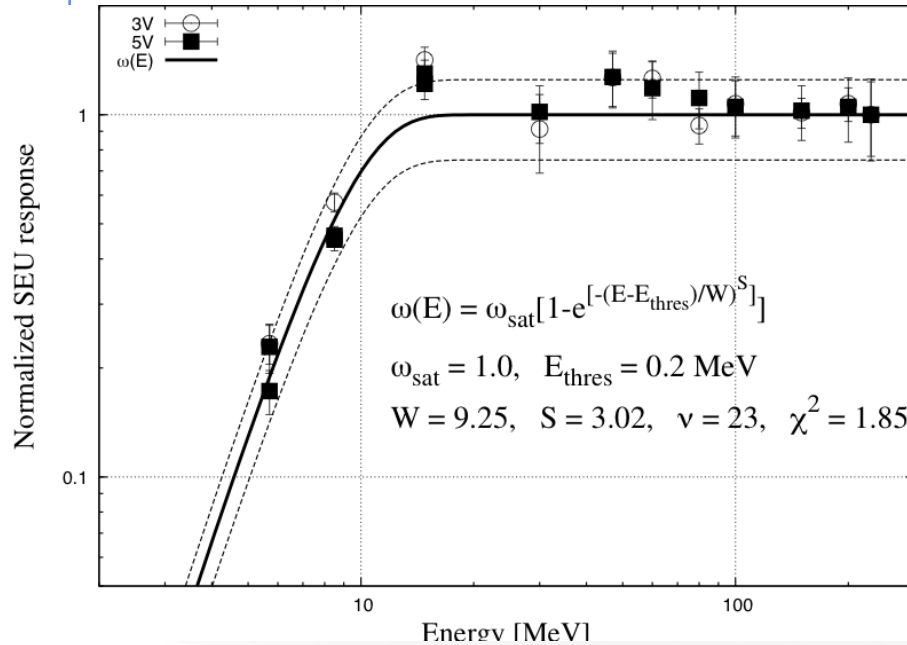


# Device response

e.g. LHC RadMon



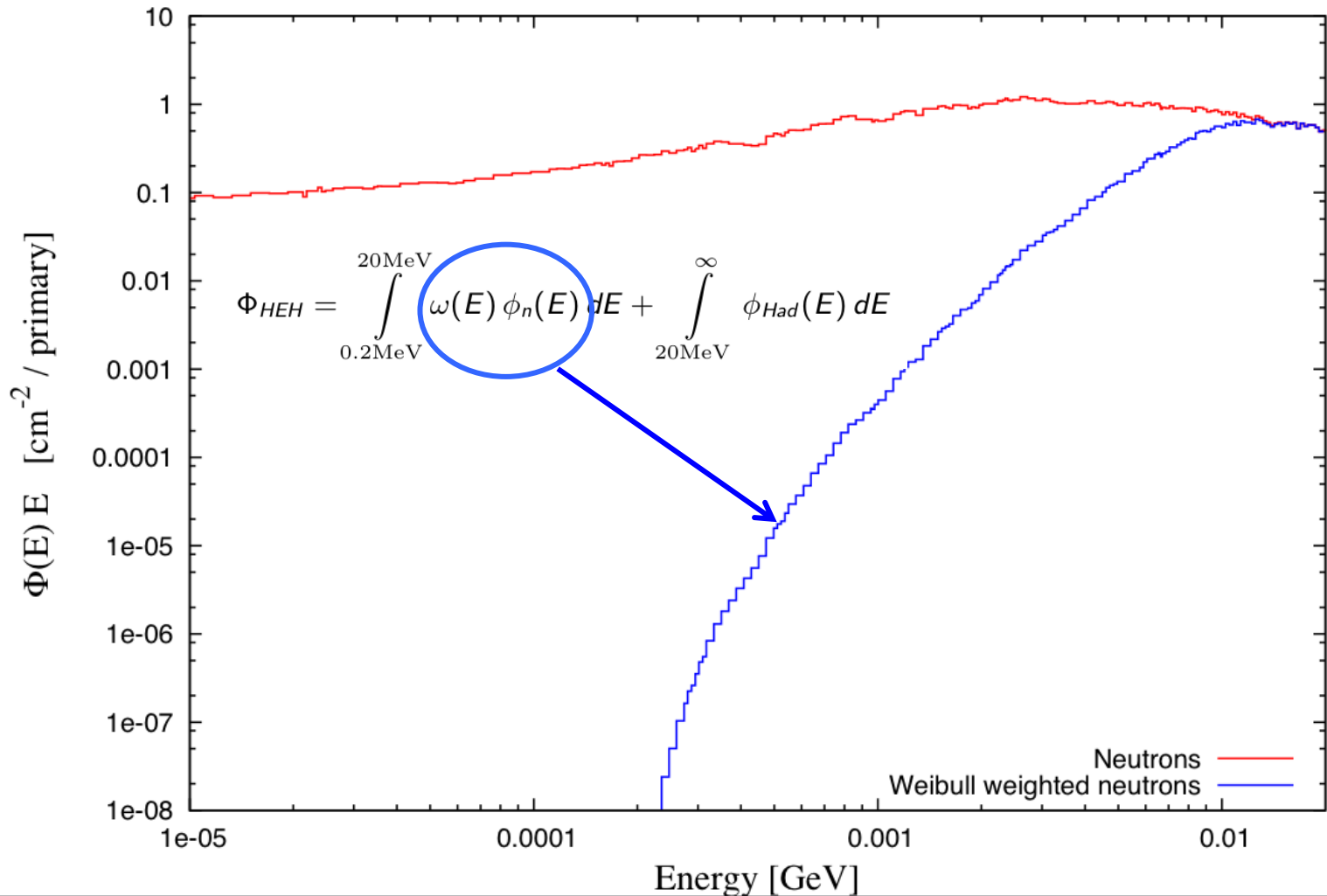
# HEHAD-EQ



$$\Phi_{HEH} = \int_{0.2\text{MeV}}^{20\text{MeV}} \omega(E) \phi_n(E) dE + \int_{20\text{MeV}}^{\infty} \phi_{Had}(E) dE$$

# HEHAD-EQ

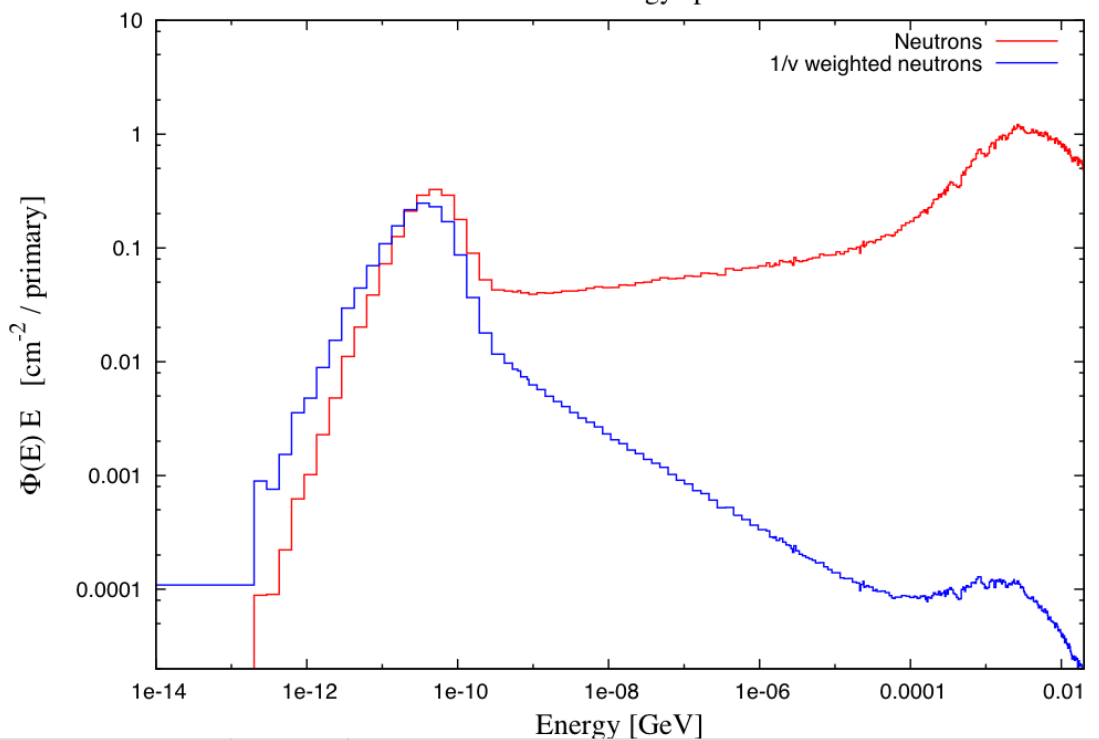
Neutron lethargy spectra



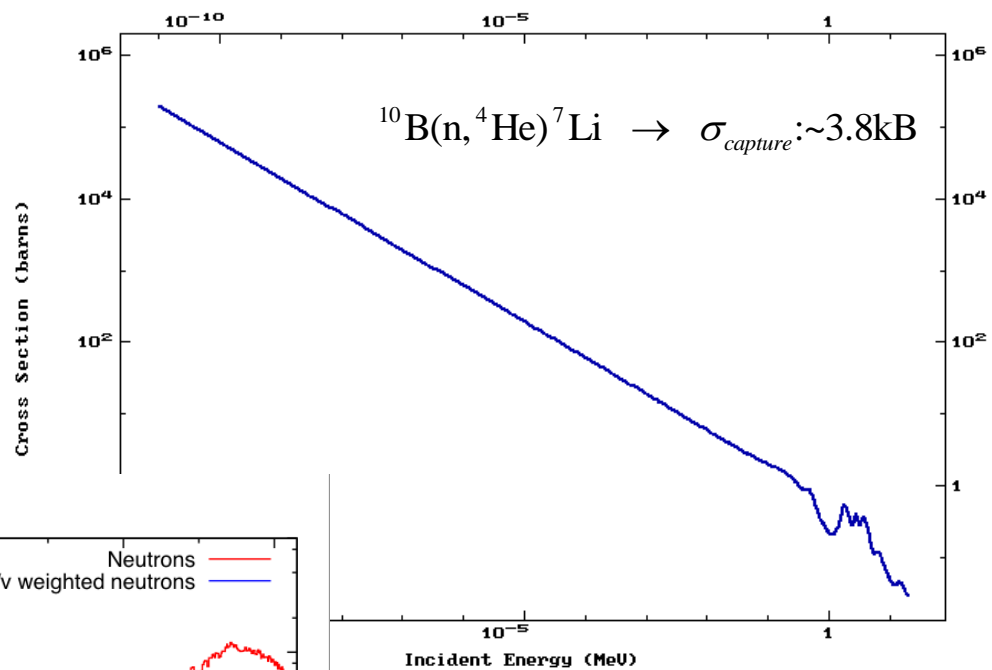
# THNEU-EQ



Neutron lethargy spectra



ENDF Request 89784, 2818-Oct-30,16:37:54



# Related Scoring CARDS & Quantities

DOSE	total ionizing dose (TID) in (obviously...)	GeV/g!
SI1MEVNE	Silicon 1 MeV-neutron equivalent fluence	
HADGT20M	Hadrons fluence with energy > 20 MeV	
HEHAD-EQ	as above, but weighted for n < 20 MeV	
THNEU-EQ	1/v weighted neutrons	

- **USRTRACK** scores average  $d\Phi/dE$  (differential fluence) in a given region (SI1MEVNE, HADGT20M or any particle type)
- **USRBDX** scores for the same quantities average  $d^2\Phi/dE d\Omega$  (double-differential fluence or current) on a given surface (between two regions)
- **USRBIN** scores the spatial distribution either of deposited dose, or fluence (1MeV or 20MeV) in a regular mesh (cylindrical or Cartesian) described by the user
- **USRBIN** also scores the same quantities on a region basis

\* 1) high-energy hadron fluence spectrum

```
USRTRACK      -1.  HADGT20M      -31.  RADMON1      125.  170.Ust20MeV
USRTRACK      1D3    1D-14
&
```

\* 2) displacement damage spectrum

```
USRBDX        98.  SI1MEVNE      -41.  TAIR  RADMON1  150.Usx1MeV
USRBDX        1D3    1D-14      170.  &
```

\* 3) dose distribution in a regular mesh through the geometry

```
USRBIN        10.  DOSE          -21.  100.  20.  200.UsbDose
USRBIN       -100. -20.  -100.  100.  20.  150.&
```

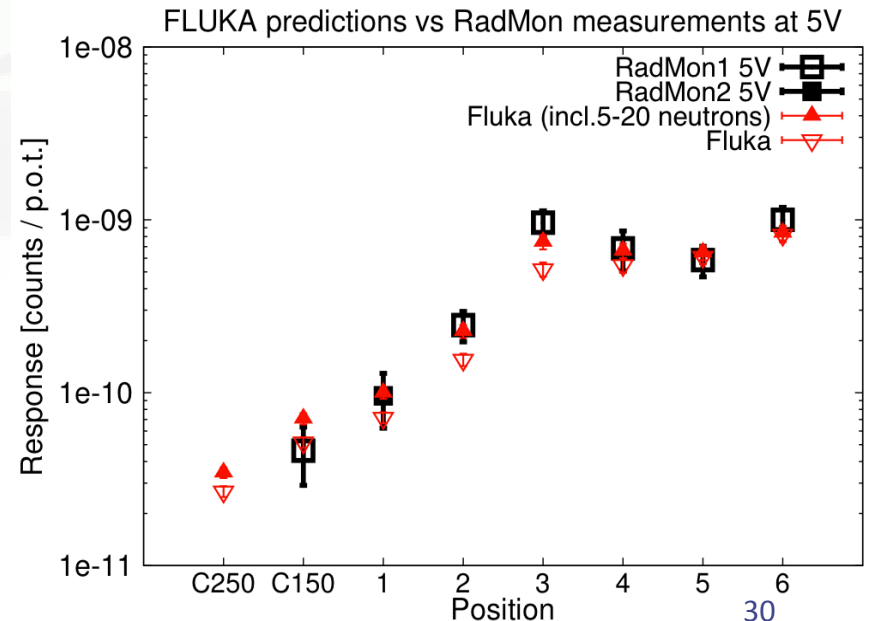
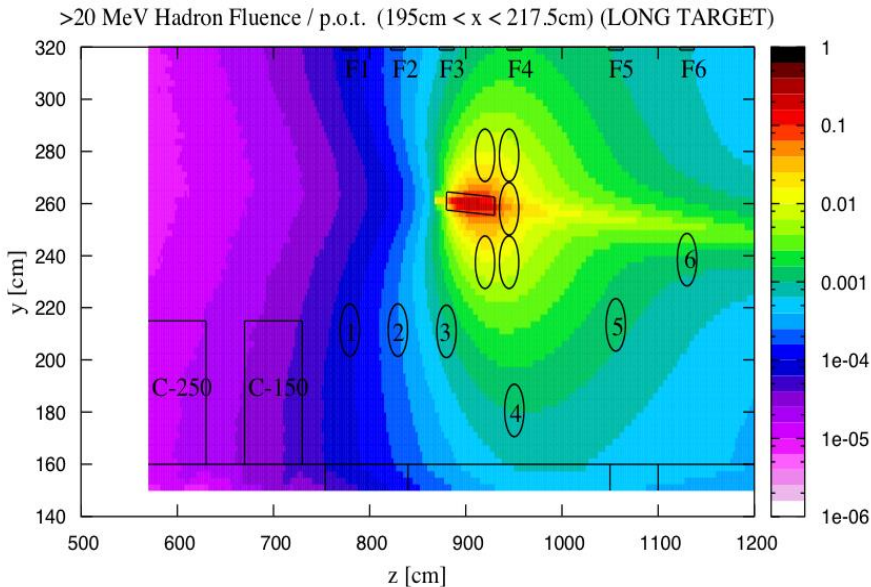
\* 4) integrated high-energy hadron equivalent fluence on a region basis

```
USRBIN        18.0 HEHAD-EQ      -37.0  LSTREG  300.0  10000.0UrbReg20
USRBIN        FSTREG  0.0 -10000.0  1.0  1.0  1.0  &
```

# Application benchmark @ CERF

- Response of monitor measured in a mixed field facility and compared to predictions by Monte Carlo simulations

$$\#SEU = S_{Th. n.} \times F_{Th. n.} + \sigma_{HEH} \cdot \Phi_{HEH}$$





# Neutrons

# Reminder Neutrons

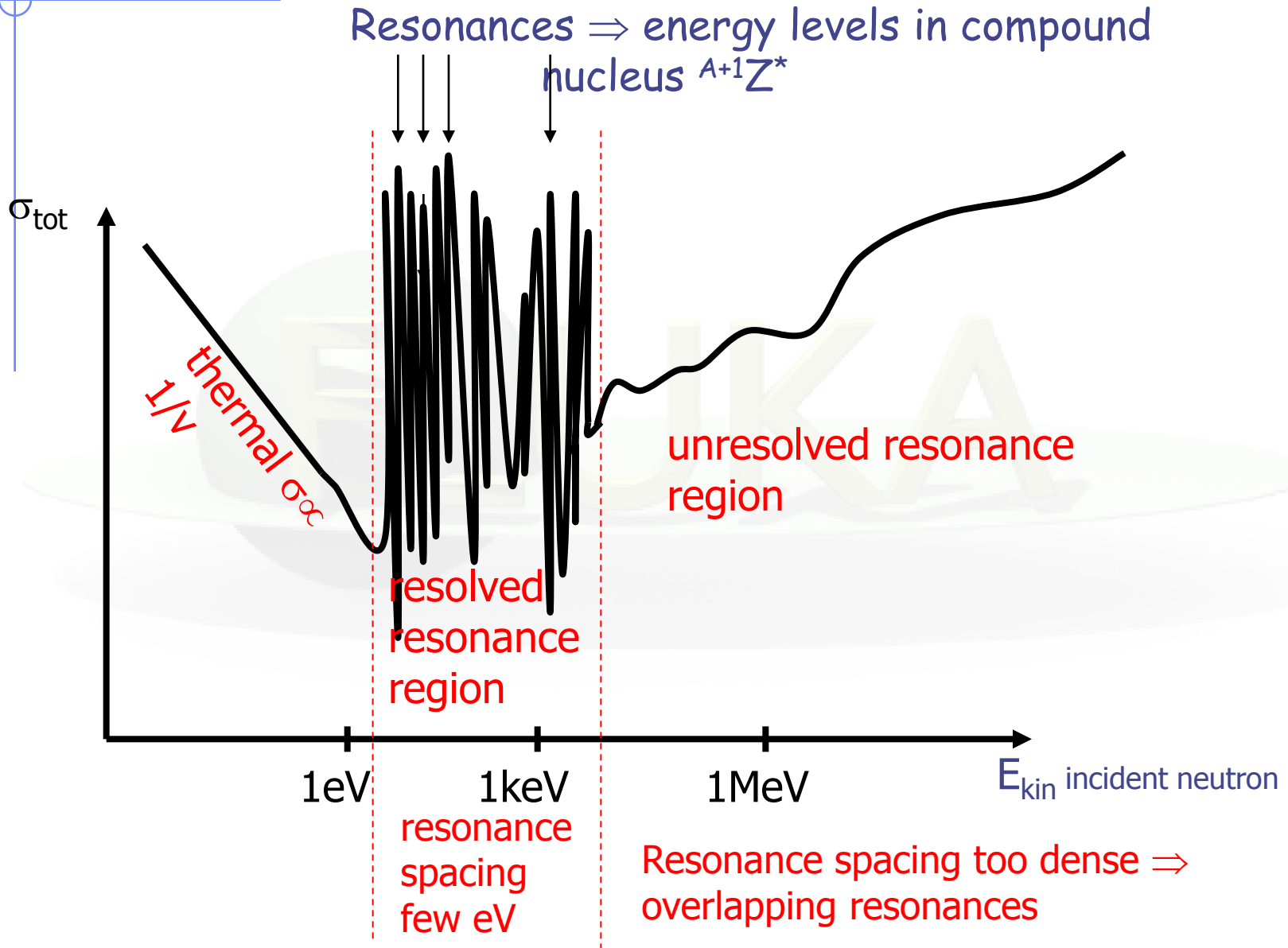
- In FLUKA we call neutrons below 20 MeV **low energy neutrons**
- Neutron interactions at higher energy are handled by FLUKA nuclear models
- Transport and interactions of neutrons with energies below 20 MeV are handled by a dedicated library

## Why are low Energy Neutrons special?

- The neutron has no charge → can interact with nuclei at low energies, e.g. meV
- Neutron cross sections ( $\sigma$ ) are complicated → cannot be calculated by models → we rely on data files



# Typical neutron cross section



# Material Correspondence: LOW-MAT

- The **LOW-MAT** card sets the correspondence between FLUKA materials and the low energy neutron cross sections
- If a material has the same name as a name given in the list of low neutron materials, the correspondence between material and low energy neutron transport is set automatically, and a **LOW-MAT** card is not necessary. The **first material** with the right name is taken. This is always a material at room temperature.
- That means that **for the predefined material HYDROGEN hydrogen bound in water is used**, not the free gas one
- If you want to use low energy neutron transport in H<sub>2</sub> gas you have to do this explicitly by a **LOW-MAT** card

# Basis: Evaluated Nuclear Data Files

- Evaluated nuclear data files (ENDF, JEFF, JENDL...)
  - typically provide neutron  $\sigma$  (cross sections) for  $E < 20\text{MeV}$  for all channels
  - $\sigma$  are stored as continuum + resonance parameters

## Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches are used: **point-wise** ("continuous" cross sections) and **group-wise** transport
- Point-wise follows cross section precisely but it can be time and memory consuming
- Group approach is widely used in neutron transport codes because it is fast and gives good results for most application

Complex programs (NJOY, PREPRO...) convert ENDF files to **point-wise or group-wise cross sections**, including Doppler broadening etc.

# FLUKA: Point-Wise Neutron Cross Sections

- ***Point-wise neutron transport*** is available for  $^1\text{H}$  (above 10 eV if bound H requested, down to  $10^{-5}$  eV otherwise) and  $^6\text{Li}$
- ***Detailed correlated reaction products*** are available for  $^1\text{H}$ ,  $^6\text{Li}$ ,  $^{10}\text{B}$  (only for the reaction  $^{10}\text{B}(n,\alpha)^7\text{Li}$ ), and the  $^{14}\text{N}(n,p)$  reaction. All reaction products are then transported explicitly according to transport setting (**PHYSICS**).
- Recoil proton production is ON by default for H and  $^{14}\text{N}(n,p)$
- while for the others and for point-wise treatment it depends on the **DEFAULT** set chosen
- Both are important for precision studies, detector response (exp. scintillators), borated materials...
- To require ***point-wise neutron transport and reaction products*** (where available), use the **LOW-NEUT** card with **WHAT(6)=1**.

# Materials with molecular binding

- Available materials with molecular bindings at 296K:
  - H (natural isotopic amount) in  $\text{H}_2\text{O}$ ,  $\text{CH}_2$
  - $^1\text{H}$  in  $\text{H}_2\text{O}$ ,  $\text{CH}_2$
  - $^2\text{D}$  in  $\text{D}_2\text{O}$
  - C in graphite
- Use of these materials makes the thermal neutron calculation more realistic and can affect the energy and spatial distributions
- Example:  $\text{CH}_2$  (polyethylene) including molecular binding
  - Create a material hydrogen and give a corresponding **LOW-MAT** card that refers to H bound in  $\text{CH}_2$
  - Give a **COMPOUND** card that creates  $\text{CH}_2$  as a compound of bound H and normal carbon
- Reminder: for hydrogen, **H bound in water is the default**, because it is the first in the list of low energy neutron materials

# Self-shielding [1/4]

- The group structure is necessarily coarse with respect to the **resonance structure** in many materials
- A resonance in a material present in a dilute mixture or as a small piece cannot affect much a smooth neutron flux (so-called “**infinite dilution**”)
- But if an isotope exhibiting large resonances is **very pure** or is present with a **large fractional abundance**, it can act as a “**neutron sink**”, causing sharp dips in the neutron spectrum corresponding to each resonance → an apparent decrease in  $\sigma$
- This effect, which results in a lower reaction rate  $\sigma\Phi$ , is called ***self-shielding*** and is necessarily **lost in the process of cross section averaging** over the width of each energy group, unless a special correction is made

# Self-shielding [2/4]

- Self-shielded materials in FLUKA:

- **$^{27}\text{Al}$**  at 296K, 87K, 4K, 430K

- **natA,  $^{40}\text{Ar}$**  at 296K, 87K

- **natFe** at 296K, 87K, 4K, 430K

- **natCu** at 296K, 87K, 4K, 430K

- **$^{181}\text{Ta}$**  at 296K, 87K

- **natW** at 296K, 87K, 4K, 430K

- **$^{197}\text{Au}$**  at 296K, 87K

- **natPb** at 296K, 87K

- **$^{208}\text{Pb}$**  at 296K

- **$^{209}\text{Bi}$**  at 296K, 87K

- ◆ Special case: **cast iron (natFe +5%C)** at 296K, 87K, 4K, 430K (see slide further on)

# Self-shielding [3/4]

- When to use these materials?
  - Bulky (huge) pieces that are very pure (containing only one isotope)
- When not to use self-shielded materials?
  - “small” iron, copper, lead, aluminum pieces
  - Thin gold foils (but a self-shielded 100 $\mu$ m Au foil is available)
  - Diluted materials
- How to use self-shielded materials?
  - Define your material with a **MATERIAL** card
  - Give additionally a **LOW-MAT** card and give the proper identifiers in WHAT(2)-WHAT(4) and SDUM
  - If you have to use self-shielded and non self-shielded materials of the same element you need to define 2 different materials
  - Attention: predefined materials like iron, copper and lead are not self-shielded, you have to give a **LOW-MAT** card to use them self-shielded



# Self-shielding [4/4]

- **Cast iron** is iron with a significant amount of carbon
- There is a self-shielded material cast iron in the low energy neutron library which is prepared to be used for creating a compound of iron and roughly 5% carbon. The amount of carbon doesn't need to be exactly 5%.
- **How to create self-shielded cast iron?**
  - Define a material iron called FeCarbSS (or any other name you like) with a **MATERIAL** card (parameters as for natural iron)
  - Insert a **LOW-MAT** card for FeCarbSS with the proper **identifiers for cast iron** in WHAT(2)-WHAT(4) and SDUM
  - Insert a **MATERIAL** card to declare a compound material called CastFe (or any other name you like)
  - Insert a **COMPOUND** card for defining CastFe as a compound of FeCarbSS and CARBON (predefined)



# Backup

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

# Factor of 2 (Kinchin & Pease)

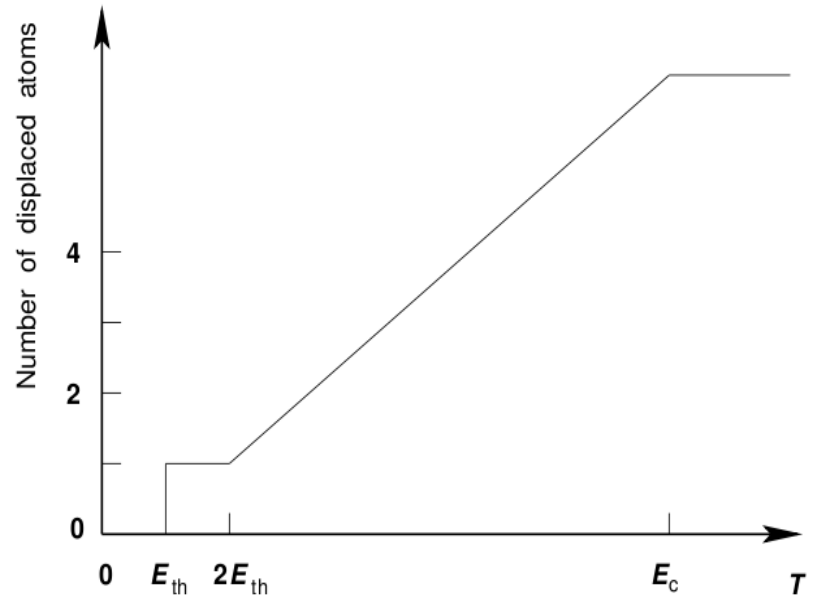
- The cascade is created by a sequence of two-body elastic collisions between atoms
- In the collision process, the energy transferred to the lattice is zero
- For all energies  $T < E_c$  electronic stopping is ignored and only atomic collisions take place. No additional displacement occur above the cut-off energy  $E_c$
- The energy transfer cross section is given by the **hard-sphere** model.

$$v(T)=0 \quad \text{for } 0 < T < E_{th} \text{ (phonons)}$$

$$v(T)=1 \quad \text{for } E_{th} < T < 2E_{th}$$

$$v(T)=T/2E_{th} \quad \text{for } 2E_{th} < T < E_c$$

$$v(T)=E_c/2E_{th} \quad \text{for } T > E_c$$



Schematic relation between the number of displaced atoms in the cascade and the kinetic energy T of the primary knock-on atom

Energy is equally shared between two atoms after the first collision  
 Compensates for the energy lost to sub threshold reactions

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

# $\kappa$ displacement efficiency

- $\kappa=0.8$  value deviates from the **hard sphere model** (K&P), and compensates for the forward scattering in the displacement cascade
- The displacement efficiency  $\kappa$  can be considered as independent of  $T$  only in the range of  $T \leq 1-2$  keV. At higher energies, the development of collision cascades results in **defect migration** and **recombination of Frenkel pairs** due to overlapping of different branches of a cascade which translates into decay of  $\kappa(T)$ .
- From molecular dynamics (MD) simulations of the primary cascade the number of surviving displacements,  $N_{MD}$ , normalized to the number of those from NRT model,  $N_{NRT}$ , decreases down to the values about 0.2–0.3 at  $T \approx 20-100$  keV. The efficiency in question only slightly depends on atomic number  $Z$  and the temperature.

$$N_{MD}/N_{NRT} = 0.3-1.3$$

$$N_{MD} / N_{NRT} = 0.3-1.3 \left( -\frac{9.57}{X} + \frac{17.1}{X^{4/3}} - \frac{8.81}{X^{5/3}} \right)$$

where  $X \equiv 20 T$  (in keV).

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

# Lindhard partition function $\xi$ [1/3]

- The partition function gives the fraction of **stopping power**  $S$  that goes to NIEL

$$\xi(T) = \frac{S_n}{S} \quad \text{where} \quad S = \frac{dE}{dx} = \frac{dE_n}{dx} + \frac{dE_e}{dx} = S_n + S_e$$

- Lindhard, Robinson assumption:

The incident particle has energy  $E$ , and due to the interactions during the slowing down the energy is transferred to atoms  $E_n$  and to electrons  $E_e$

$$E = E_e + E_n$$

The equation that has to be satisfied is

$$\int d\sigma_{ne} \left[ E_n \left( E - T_n - \sum_i T_{ei} \right) - E_n(E) + E_n(T_n - U) + \sum_i E_{ne}(T_{ei} - I_i) \right] = 0$$

where  $d\sigma_{n,e}$  are the differential cross-sections corresponding to particle scattering on nucleus and electrons,  $T_n$  ( $T_{ei}$ ) energy transfer to nucleus (electrons),  $U$  energy in atomic(lattice) binding,  $I_i$  ionization energies

$$N_F = \kappa \frac{\xi(T)T}{2E_{th}}$$

# Lindhard partition function $\xi$ [2/3]

- Approximations used: Electrons do not produce recoil nuclei with appreciable energy, lattice binding energy is neglected, etc...

$$(S_n + S_e)E'_n(E) = \int E_n(T) \frac{d\sigma_n}{dT} dT$$

where

$$S_{ne}(E) = \int T_{ne} d\sigma_{ne}$$

- approximated to

$$\xi(T) = \frac{1}{1 + F_L \cdot (3.4008 \cdot \varepsilon(T)^{1/6} + 0.40244 \cdot \varepsilon(T)^{3/4} + \varepsilon(T))}$$

$$F_L = 30.724 \cdot Z_1 \cdot Z_2 \sqrt{Z_1^{2/3} + Z_2^{2/3}}$$

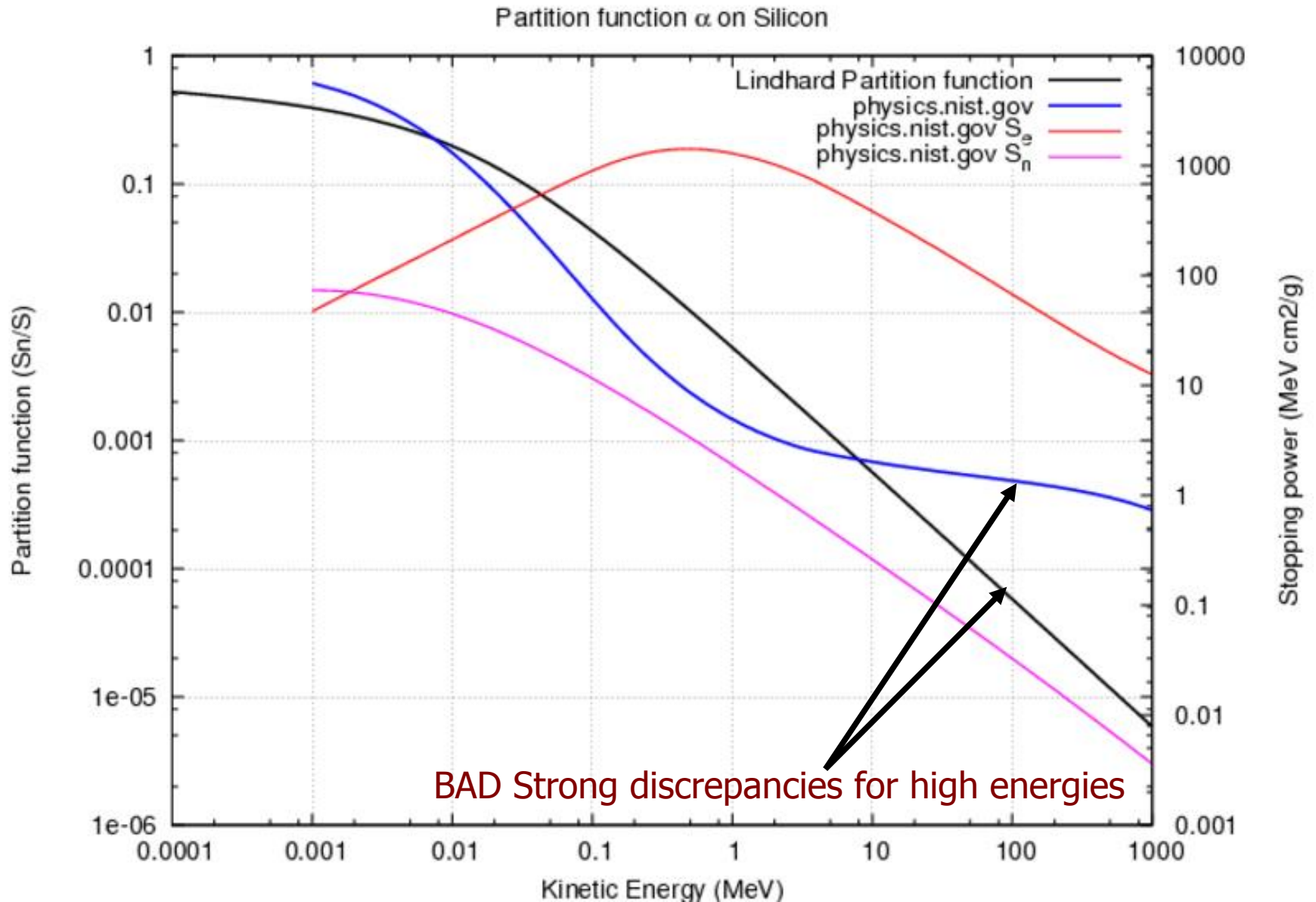
$$\varepsilon(T) = \frac{T}{0.0793 \frac{Z_1^{2/3} \cdot \sqrt{Z_2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4}} \cdot \frac{(A_1 + A_2)^{3/2}}{A_1^{3/2} \sqrt{A_2}}}$$

Z,A	charge and mass
1	projectile
2	medium
T	recoil energy (eV)

Nice feature: It can handle any projectile  $Z_1, A_1$  whichever charged particle

# Lindhard partition function $\xi$ [3/3]

$$N_F = \kappa \frac{\xi(T) T}{2E_{th}}$$



# Restricted Nuclear Stopping Power

- Lindhard approximation uses the **unrestricted NIEL**. Including all the energy losses also those below the threshold  $E_{th}$
- FLUKA is using a more accurate way by employing the **restricted nuclear losses**

$$S(E, E_{th}) = N \int_{E_{th}}^{\gamma E} T \left( \frac{d\sigma}{dT} \right) dT$$

where:

$S(E, E_{th})$  is the restricted energy loss

$N$  atomic density

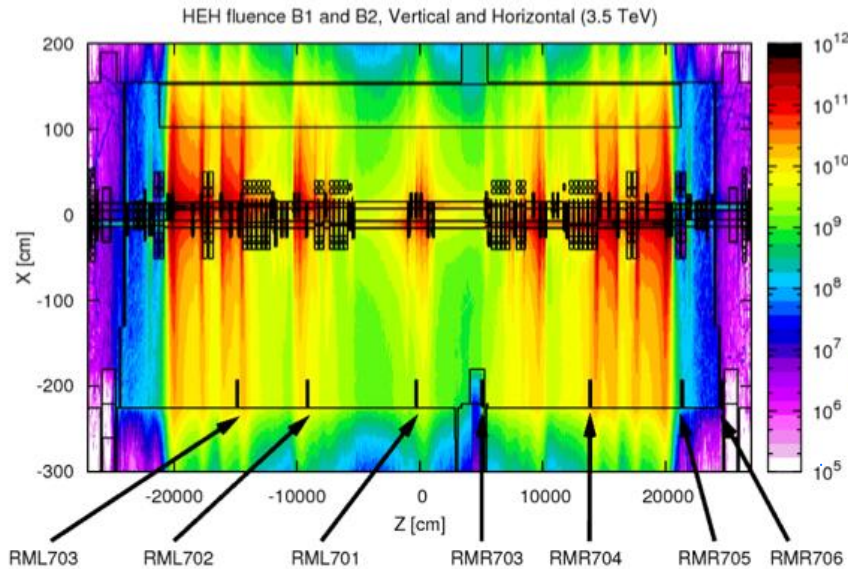
$T$  energy transfer during ion-solid interaction

$d\sigma/dT$  differential scattering cross section

$\gamma = \frac{4M_1M_2}{(M_1 + M_2)^2}$  maximum fraction of energy transfer during collision



# App. benchmark: IR7 collimation region



- 3.5 TeV proton beams of opposite direction
- Interacts with collimators → radiation showers
  - Interactions and transport by FLUKA
- RadMons mounted along the wall (5V)
- Complicated beam line geometry (> 500 m)
- Sim. results normalized to 2010 operation

## Margins to be considered:

- Simulation: x2-3 (geometry, material, positioning, loss distribution, model)
- Normalization: 50%

## Results for LHC operation in 2010

RadMon	Meas.	Err [%]	FLUKA	Err [%]	F/M	Err [%]
RML703	13246	1	13800	19	<b>1.0</b>	20
RML702	4601	2	7650	20	<b>1.7</b>	30
RML701	2406	2	3590	20	<b>1.5</b>	30
RMR703	878	29	641	20	<b>0.7</b>	20
RMR704	17903	3	17600	20	<b>1.0</b>	20
RMR705	264	6	731	18	<b>2.8</b>	50
RMR706	13	23	7	29	<b>0.6</b>	20

Err.: statistical / counting & variation in  $\sigma_{SEU}$ .

